L4 4 L3

=> d l4 1-4 bib abs hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2001:354666 CAPLUS

DN 135:137481

TI Synthesis of some new 1,5-benzothiazepines containing 2H-1-benzopyran-2-one heterocycle

AU Prashant, A.; Rao, S. Srinivas; Chowdary, K. S.; Krishnan, V. S. H.

CS Dr. Krishnan's Laboratories, Hyderabad, 072, India

SO Heterocyclic Communications (2001), 7(1), 61-66 CODEN: HCOMEX; ISSN: 0793-0283

Ι

PB Freund Publishing House Ltd.

DT Journal

LA English

OS CASREACT 135:137481

GI

AB A facile procedure was developed for the synthesis of 2-aryl/heteryl-4-(2H-1-benzopyran-2-on-8-yl)-2,3-dihydro-1,5-benzothiazepines I [R = H, Me; R1 = Ph, 4-MeOC6H4, 2-thienyl, 3-O2NC6H4, 4-ClC6H4, 4-Me2NC6H4, 4-HO-3-MeOC6H3, 3,4-(MeO)2C6H3, 3-pyridyl; R2 = H, Cl 5a-o] in 50-70% yields by the cyclocondensation reaction of 1-(2H-1-benzopyran-2-one-8-yl)-3-aryl/heteryl-2-propenones with 2-amino-5-R2-thiophenols (R2 = H 4a Cl 4b) in toluene in the presence of trifluoroacetic acid.

IT 79692-52-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and cyclocondensation reaction of, with aminothiophenols)

RN 79692-52-7 CAPLUS

CN 2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-8-[1-oxo-3-(3-pyridinyl)-2-propenyl]- (9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
applicants' own
      ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
L4
AN
      2001:185740 CAPLUS
DN
      134:222628
      Preparation of 8-(arylpropenoyl) coumarins as antiproliferative agents
TI
      Bombardelli, Ezio; Valenti, Piero
IN
PA
      Indena S.p.A., Italy
      PCT Int. Appl., 31 pp.
SO
      CODEN: PIXXD2
DT
      Patent
      English
LA
FAN.CNT 1
                                                     APPLICATION NO.
      PATENT NO.
                           KIND
                                  DATE
                                                                          DATE
                                                    WO 2000-EP8367
ΡI
      WO 2001017984
                           A1
                                  20010315
                                                                          20000828
               AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
               CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
                SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
           RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
                CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                   EP 2000-965902
                                                                          20000828
                            A1
                                  20020612
      EP 1212311
                                  20030326
      EP 1212311
                            В1
               AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, LT, LV, FI, RO, MK, CY, AL
                                                     JP 2001-521731
                                                                          20000828
      JP 2003508523
                            T_2
                                  20030304
                                                     AT 2000-965902
                                                                          20000828
                                  20030415
      AT 235480
                            Ε
                                                     US 2002-75625
                                                                          20020215
                                  20021031
      US 2002161036
                            A1 ·
                                  20020503
                                                     NO 2002-1048
                                                                          20020301
      NO 2002001048
                            Α
PRAI GB 999-20908
                            Α
                                  19990903
      WO 2000 -EP8367
                            W
                                  20000828
os
      MARPAT 134:222628
GΙ
```

The title chalcone coumarins (I) [wherein Ar = (un)substituted (hetero)aryl; R = OH, OR10, or OCOR11; R10 = (un)substituted alkyl, alkenyl, or alkynyl; R11 = alkyl, alkenyl, alkynyl, or Ph; R1 = H or (un)substituted alkyl] were prepd. as antiproliferative agents for the treatment or prevention of neoplasms, particularly those located in the uterus, ovary, or breast. For example, coupling pyridine-3-carboxaldehyde with 4-methyl-7-(3-methylbut-2-enyloxy)-8-acetylcoumarin in KOH and EtOH afforded II, which reduced the IC50 of paclitaxel from 426 nM to 86 nM against drug-resistant breast cancer cells in a cytotoxicity assay. I may also be useful for the treatment or prevention of menopausal disorders and osteoporosis (no data).

329366-37-2P, 1-[4-Methyl-7-(3-methylbut-2-enyloxy)coumarin-8-yl]3-(pyridine-3-yl)propen-1-one 329366-41-8P, 1-[4-Methyl-7-(2-methylallyloxy)coumarin-8-yl]-3-(pyridine-3-yl)propen-1-one
329366-47-4P, 1-[4-Methyl-7-(allyloxy)coumarin-8-yl]-3-(pyridin-3-yl)propen-1-one

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 8-(arylpropenoyl) coumarin antiproliferative agents by coupling 8-acetylcoumarins with arylaldehydes)

RN 329366-37-2 CAPLUS

CN 2H-1-Benzopyran-2-one, 4-methyl-7-[(3-methyl-2-butenyl)oxy]-8-[1-oxo-3-(3-pyridinyl)-2-propenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & \\ \text{CH} & \\ & \\ \text{C$$

329366-41-8 CAPLUS

RN

CN 2H-1-Benzopyran-2-one, 4-methyl-7-[(2-methyl-2-propenyl)oxy]-8-[1-oxo-3-(3-pyridinyl)-2-propenyl]- (9CI) (CA INDEX NAME)

AB The title compds. I (R = H, OH; R1 = H, Et), II (R = H, OH), and III (R = H, OH; R2 = H, Me) were prepd. from the corresponding o-hydroxyacetyl coumarin. Thus, 7-hydroxy-8-acetyl-4-Me coumarin was condensed with 3-pyridinecarboxaldehyde and the product cyclized by SeO2 to give I (R = R1 = H).

IT 79692-52-7P 79692-53-8P 79692-54-9P 79692-55-0P 79692-56-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and cyclization of, pyranocoumarin deriv. from)

RN 79692-52-7 CAPLUS

CN 2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-8-[1-oxo-3-(3-pyridinyl)-2-propenyl]- (9CI) (CA INDEX NAME)

RN 79692-53-8 CAPLUS

CN 2H-1-Benzopyran-2-one, 6-ethyl-7-hydroxy-4-methyl-8-[1-oxo-3-(3-pyridinyl)-2-propenyl]- (9CI) (CA INDEX NAME)

CODEN: FRXXBL

DT Patent LA French

FAN.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
рт	FR 2387956	 Δ1	 19781117	FR 1977-11871	19770420
	FR 2387956	B1	19810109	FR 1,9//-110/1	. 13//0420
PRAI	FR 1977-11871		19770420		

GΙ

AB Pyridines I (R = R1 = H, RR1 = bond; R2 = substituted Ph, pyridyl, thienyl, furyl, benzofuranyl, styryl, quinolinyl; X = CO, CHOH, CH2, C:NOH) were prepd.; they were useful in the treatment of hypoxia, decreased resistance to blood circulation in capillary vessels, increased capillary vessel permeability, and were coronary vasodilators.

4-Formylpyridine in 1% NaOH at room temp. was treated with 2,3,4-(MeO)3C6H2COMe in EtOH to give I [RR1 = bond, R2 = 2,3,4-(MeO)3C6H2, X = CO](II). II at 30 mg/kg increased the survival rate of rats at 150 mm Hg 24%.

IT 72512-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and treatment of anoxia by)

RN 72512-20-0 CAPLUS

CN 2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-8-[1-oxo-3-(4-pyridinyl)-2-propenyl]- (9CI) (CA INDEX NAME)

Structures 9 10/075675

=> d bib abs

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ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
L2
       2001:185740 CAPLUS
AN
DN
       134:222628
       Preparation of 8-(arylpropenoyl) coumarins as antiproliferative agents
ΤI
       Bombardelli, Ezio; Valenti, Piero
IN
PA
       Indena S.p.A., Italy
       PCT Int. Appl., 31 pp.
SO
       CODEN: PIXXD2
DT
       Patent
LΑ
       English
FAN.CNT 1
                                                                  APPLICATION NO. DATE
       PATENT NO.
                                  KIND DATE
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                                          _____
                                                                  ______
                                                                  WO 2000-EP8367
       WO 2001017984
                                  A1
                                           20010315
                                                                                             20000828 <--
PΙ
             W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                                 EP 2000-965902
       EP 1212311
                                   A1
                                           20020612
       EP 1212311
                                   B1
                                           20030326
                  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                    IE, SI, LT, LV, FI, RO, MK, CY, AL
       JP 2003508523
                                   Т2
                                           20030304
                                                                  JP 2001-521731
                                                                                             20000828
                                           20021031
                                                                  US 2002-75625
                                                                                             20020215
       US 2002161036
                                   A1
                                           20020503
                                                                  NO 2002-1048
                                                                                             20020301
       NO 2002001048
                                   Α
PRAI GB 1999-20908
                                           19990903
                                   Α
       WO 2000-EP8367
                                   W
                                           20000828
OS
       MARPAT 134:222628
GI
```

The title chalcone coumarins (I) [wherein Ar = (un) substituted (hetero) aryl; R = OH, OR10, or OCOR11; R10 = (un) substituted alkyl, alkenyl, or alkynyl; R11 = alkyl, alkenyl, alkynyl, or Ph; R1 = H or (un) substituted alkyl] were prepd. as antiproliferative agents for the treatment or prevention of neoplasms, particularly those located in the uterus, ovary, or breast. For example, coupling pyridine-3-carboxaldehyde with 4-methyl-7-(3-methylbut-2-enyloxy)-8-acetylcoumarin in KOH and EtOH

afforded II, which reduced the IC50 of paclitaxel from 426 nM to 86 nM against drug-resistant breast cancer cells in a cytotoxicity assay. I may also be useful for the treatment or prevention of menopausal disorders and osteoporosis (no data).

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 8-[3-(3-methoxyphenyl)-1-oxo-2-propenyl]-4-methyl-7-(2-propynyloxy)- (9CI)

MF C23 H18 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):33

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 4-methyl-8-[1-oxo-3-(3-pyridinyl)-2-propenyl]-7-(2-

propenyloxy) - (9CI)

MF C21 H17 N O4

$$H_{2}C = CH - CH_{2} - O$$

$$Me$$

$$CH$$

$$CH$$

$$C = O$$

$$C = O$$

$$Me$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 4-methyl-7-[(3-methyl-2-butenyl)oxy]-8-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl]- (9CI)

- L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS
- IN Benzaldehyde, 3-methoxy- (9CI)
- MF C8 H8 O2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS
- IN Benzaldehyde, 2,6-dichloro- (6CI, 7CI, 8CI, 9CI)
- MF C7 H4 Cl2 O
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS
- IN 2H-1-Benzopyran-2-one, 4-methyl-8-[1-oxo-3-(3-pyridinyl)propyl]-7-(2-propynyloxy)- (9CI)

$$CH_2$$
 CH_2
 CH_2

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 4-methyl-8-(1-oxo-3-phenyl-2-propenyl)-7-(2-IN propenyloxy) - (9CI)

C22 H18 O4 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 4-methyl-7-[(3-methyl-2-butenyl)oxy]-8-(1-oxo-3-IN

phenyl-2-propenyl)- (9CI)

MF C24 H22 O4

REGISTRY COPYRIGHT 2003 ACS L334 ANSWERS

3-Pyridinecarboxaldehyde (9CI) IN

C6 H5 N O MF

COM CI

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 8-[3-(2,6-dichlorophenyl)-1-oxo-2-propenyl]-4-IN methyl-7-(2-propenyloxy)- (9CI)

C22 H16 Cl2 O4 MF

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ \text{CH} & & \\ \text{O} & & \\ \text{Me} & & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2003 ACS L3 34 ANSWERS

2H-1-Benzopyran-2-one, 4-methyl-8-(1-oxo-3-phenyl-2-propenyl)-7-(2-IN propynyloxy) - (9CI)

MF C22 H16 O4

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 4-methyl-7-[(2-methyl-2-propenyl)oxy]-8-[1-oxo-3-IN (3,4,5-trimethoxyphenyl)propyl] - (9CI)

MFC26 H28 O7

$$\begin{array}{c} \text{OMe} \\ \text{MeO} & \text{OMe} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{Me} - \text{C} - \text{CH}_2 - \text{O} \\ \text{Me} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2003 ACS L3 34 ANSWERS

2H-1-Benzopyran-2-one, 8-acetyl-4-methyl-7-[(3-methyl-2-butenyl)oxy]-IN (9CI)

C17 H18 O4 MF

$$\mathsf{Me_2C} = \mathsf{CH} - \mathsf{CH_2} - \mathsf{O} \qquad \qquad \mathsf{Ne}$$

$$Me_2C = CH - CH_2 - O \qquad AC \qquad O \qquad O$$

$$Me \qquad Me$$

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzaldehyde, 4-fluoro- (9CI)

MF C7 H5 F O

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 8-acetyl-7-methoxy-3-methyl- (9CI)

MF C13 H12 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 8-acetyl-4-methyl-7-(2-propynyloxy)- (9CI)

MF C15 H12 O4

$$HC \equiv C - CH_2 - O$$
 Me
 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 8-[3-(3-methoxyphenyl)-1-oxo-2-propenyl]-4-methyl-7-IN [(2-methyl-2-propenyl)oxy] - (9CI)

C24 H22 O5 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2003 ACS 34 ANSWERS L3

2H-1-Benzopyran-2-one, 4-methyl-7-[(3-methyl-2-butenyl)oxy]-8-[1-oxo-3-(3-IN pyridinyl)-2-propenyl]- (9CI)

C23 H21 N O4 MF

$$Me_2C$$
 CH CH₂ O Me_2 CH O Me_2 CH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2003 ACS L334 ANSWERS

IN Benzaldehyde, 4-chloro- (9CI)

MF C7 H5 Cl O

CI COM

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 7-methoxy-3-methyl-8-[1-oxo-3-(2-thienyl)-2-IN propenyl] - (9CI) C18 H14 O4 S

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 4-methyl-8-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-IN

propenyl] -7-(2-propynyloxy) - (9CI)

MF C25 H22 O7

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 4-methyl-7-[(2-methyl-2-propenyl)oxy]-8-(1-oxo-3-IN phenyl-2-propenyl) - (9CI)

MF C23 H20 O4

$$\begin{array}{c} \text{CH}_2 \\ \parallel \\ \text{Me-C-CH}_2 - \text{O} \\ \end{array} \begin{array}{c} \text{C-CH-CH-Ph} \\ \text{O} \\ \text{Me} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS
Benzenepropanoic acid, .beta.-[[(1,1-dimethylethoxy)carbonyl]amino]-IN .alpha.-hydroxy-, (2aR, 4S, 4aS, 6R, 9S, 11S, 12S, 12aR, 12bS) -12b-(acetyloxy) -12-(benzoyloxy) -2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1Hcyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI)

MF C43 H53 N O14

CI COM

Absolute stereochemistry.

REGISTRY COPYRIGHT 2003 ACS 34 ANSWERS L3

2-Pyridinecarboxylic acid (9CI) IN

C6 H5 N O2 MF

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 8-[3-(4-fluorophenyl)-1-oxo-2-propenyl]-4-methyl-7-IN

(2-propynyloxy) - (9CI)

C22 H15 F O4 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

IN 2H-1-Benzopyran-2-one, 4-methyl-3-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2propenyl]-7-(2-propenyloxy)- (9CI)
MF C25 H24 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

MF C16 H16 O4

$$\begin{array}{c|c} CH_2 & Ac \\ Me-C-CH_2-O & O \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 8-acetyl-4-methyl-7-(2-propenyloxy)- (9CI)

MF C15 H14 O4

$$H_2C = CH - CH_2 - O$$

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI)

MF C5 H4 O S

CI COM

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS L3

2H-1-Benzopyran-2-one, 8-[3-(4-chlorophenyl)-1-oxo-2-propenyl]-4-methyl-7-IN (2-propenyloxy) - (9CI)

C22 H17 Cl O4 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 8-[3-(3-methoxyphenyl)-1-oxo-2-propenyl]-4-methyl-7-IN

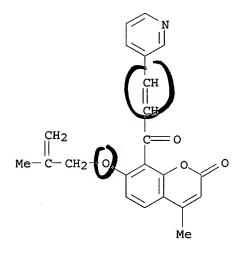
(2-propenyloxy) - (9CI)

C23 H20 O5 MF

L3

34 ANSWERS REGISTRY COPYRIGHT 2003 ACS 2H-1-Benzopyran-2-one, 4-methyl-7-[(2-methyl-2-propenyl)oxy]-8-[1-oxo-3-(3-INpyridinyl) - 2 - propenyl] - (9CI)

C22 H19 N O4 MF



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2003 ACS L3 34 ANSWERS

Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, IN (2aR, 4S, 4aS, 6R, 9S, 11S, 12S, 12aR, 12bS) -6, 12b-bis (acetyloxy) -12-(benzoyloxy) -2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI)

MF C47 H51 N O14

CI COM

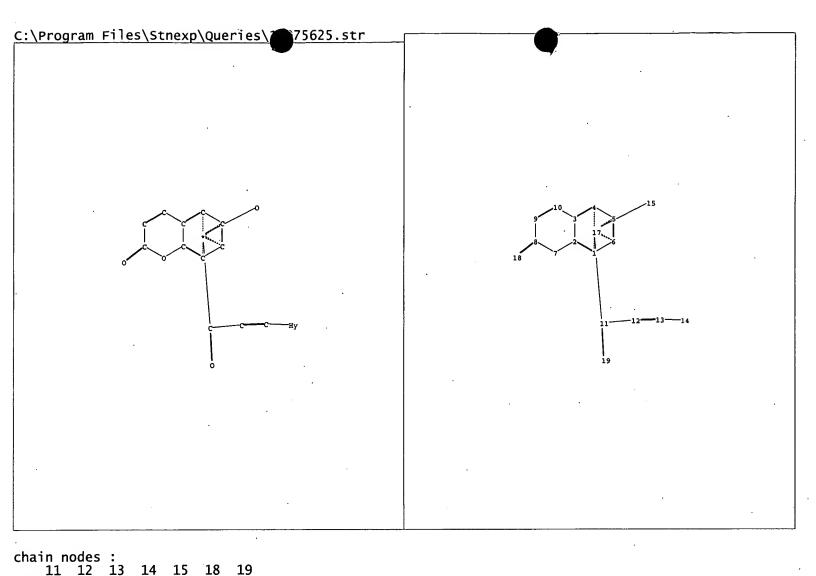
Absolute stereochemistry. Rotation (-).

L3 34 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzaldehyde, 3,4,5-trimethoxy- (6CI, 7CI, 8CI, 9CI)

MF C10 H12 O4

CI COM



```
8-18 11-12 11-19 12-13 13-14
ring bonds :
    1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10
exact/norm bonds :
    8-18 11-19 13-14
exact bonds:
    2-7 3-10 7-8 8-9 9-10 11-12 12-13
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
    containing 1:
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
Element Count:
    Node 14: Limited
        C,C5
        N,N1
```

10

ring nodes: 1 2 3 4 5 6 7

chain bonds :